

Dynamical Quasi-Stationary States in a system with long-range forces

V. Latora* and A. Rapisarda†

*Dipartimento di Fisica e Astronomia, Università di Catania,
and INFN sezione di Catania, Corso Italia 57 I 95129 Catania, Italy*
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The Hamiltonian Mean Field model describes a system of N fully-coupled particles showing a second-order phase transition as a function of the energy. The dynamics of the model presents interesting features in a small energy region below the critical point. In particular, when the particles are prepared in a “water bag” initial state, the relaxation to equilibrium is very slow. In the transient time the system lives in a dynamical quasi-stationary state and exhibits anomalous (enhanced) diffusion and Lévy walks. In this paper we study temperature and velocity distribution of the quasi-stationary state and we show that the lifetime of such a state increases with N . In particular when the $N \rightarrow \infty$ limit is taken before the $t \rightarrow \infty$ limit, the results obtained are different from the expected canonical predictions. This scenario seems to confirm a recent conjecture proposed by C.Tsallis.

I. INTRODUCTION

The Hamiltonian Mean Field (HMF) model describes N classical particles moving on the unit circle and interacting through an infinite range potential [1]. HMF has been recently studied both analytically and numerically [2–6]. The model has the advantage of having an exact solution in the canonical ensemble and therefore allows to study microscopic dynamics in connection to thermodynamic macroscopic features. The analytical calculation in the canonical ensemble predicts a second-order phase transition from a clustered phase to a “gaseous” one, where the particles are homogeneously distributed on the circle. A microcanonical solution, recently obtained, has been discussed by S.Ruffo at this conference [6]. The numerical simulations show that the dynamics is chaotic and the Lyapunov exponents are maximal at the critical point. In the energy range close to the critical point the relaxation to equilibrium is very slow, though the dynamics is strongly chaotic. In particular when the system is started in out-of-equilibrium initial conditions it shows the presence of Quasi-Stationary States (QSS) whose relaxation time increases with the size of the system. The particle motion is superdiffusive in the transient quasi-stationary regime preceding equilibration.

In the following sections we remind the reader the details of the model and then we focus on the quasi-stationary states discussing superdiffusion, velocity distributions and lifetimes. As a main result we show that close to the critical point, if the continuum ($N \rightarrow \infty$) limit is performed before the $t \rightarrow \infty$ limit, canonical equilibrium is never reached and quasi-stationary superdiffusive states live forever.

II. THE MODEL

The Hamiltonian of our system is :

$$H(\theta, p) = K + V , \quad (1)$$

where

$$K = \sum_{i=1}^N \frac{p_i^2}{2} , \quad V = \frac{1}{2N} \sum_{i,j=1}^N [1 - \cos(\theta_i - \theta_j)] \quad (2)$$

are the kinetic and potential energy. The system consists of N classical particles moving on the unit circle: each particle is characterized by the angles θ_i and the conjugate momenta p_i , and interacts with all the others. One can

*E-mail: vito.latora@ct.infn.it

†E-mail: andrea.rapisarda@ct.infn.it

also see the model in a different way: if we consider a spin vector associated to each particle $\mathbf{m}_i = [\cos(\theta_i), \sin(\theta_i)]$, the Hamiltonian then describes a linear chain of N classical fully-coupled spins, similarly to the XY model. With this interpretation we can define a total magnetization $\mathbf{M} = \frac{1}{N} \sum_{i=1}^N \mathbf{m}_i$. Thus the system is a ferromagnet at low energy and shows a second-order phase transition at the critical energy density $U_c = 0.75$ ($U = E/N$), corresponding to the critical temperature $T_c = 0.5$ in the canonical ensemble [1–3]. On the other hand, one gets an antiferromagnetic behavior by changing the sign of the interaction. This case has been studied in detail too [1,5,7].

Considering the components of the magnetization vector $\mathbf{M} = (M_x, M_y)$ and expressing the potential in the following way

$$V = \frac{N}{2}(1 - M_x^2 + M_y^2) = \frac{N}{2}(1 - M^2) \quad , \quad (3)$$

the equations of motion for the N particles are

$$\dot{\theta}_i = p_i \quad , \quad \dot{p}_i = -\sin(\theta_i)M_x + \cos(\theta_i)M_y \quad , \quad i = 1, \dots, N \quad . \quad (4)$$

The latter equations can be also recast in the form

$$\dot{\theta}_i = p_i \quad , \quad \dot{p}_i = -M \sin(\theta_i - \phi) \quad , \quad i = 1, \dots, N \quad , \quad (5)$$

where (M, ϕ) are respectively the modulus and the phase of the total magnetization vector \mathbf{M} . These equations are formally equivalent to those of a perturbed pendulum. The equations of motion were integrated numerically by means of a 4th order symplectic algorithm [8] which allowed, using a time step $\delta t = 0.2$, very long integration times (the average number of steps was of the order of 10^7) with a relative error in the total conserved energy smaller than $\Delta E/E = 10^{-5}$ (the details can be found in Refs [2,3]). Such long integration time is necessary in order to reach equilibration when out-of-equilibrium initial conditions are used. In the following we present numerical simulations for systems with different N values and energies $U = E/N$. In particular we focus on the region below the critical point.

III. LÉVY WALKS, SUPERDIFFUSION AND QUASI-STATIONARY STATES

In this section we discuss the transport properties of single particles in the transient out-of-equilibrium regime for $0.6 \leq U < U_c$ and we study the characteristics of the quasi-stationary macroscopic states. Diffusion and transport of a particle in a medium or in a fluid flow are characterized by the mean square displacement $\sigma^2(t)$, which in the long-time limit, is given by the equation

$$\sigma^2(t) \sim t^\alpha \quad , \quad (6)$$

with $\alpha = 1$ for normal diffusion. When $\alpha \neq 1$ one has anomalous diffusion, and in particular *subdiffusion* if $0 < \alpha < 1$ and *superdiffusion* if $1 < \alpha < 2$. Anomalous diffusion has been mainly studied in chaotic systems with only a few degrees of freedom [9,10], and only recently in high-dimensional systems [11,12]. In order to study the non-equilibrium properties of HMF model, we start our system in a “water bag”, i.e. an initial condition obtained by putting all the particles at $\theta_i = 0$ and giving them a uniform distribution of momenta with a finite width centered around zero. By following the dynamics of each particle, we compute the variance in the angle θ according to the expression

$$\sigma^2(t) = \langle (\theta - \langle \theta \rangle)^2 \rangle \quad , \quad (7)$$

where $\langle \cdot \rangle$ indicates the average over the N particles, and we fit the value of the exponent α in Eq. (6). In fig. 1 we show the typical motion of a particle as a function of time for a system with $N = 1000$ and $U = 0.69$. In (a) we report the time evolution of the angle and in (b) the respective momentum time evolution. It is clearly visible that the particle is sometimes trapped by the main cluster (formed by all the other particles) and oscillates around it with zero average momentum. But the particle can also frequently experience free walks in angle, with an average momentum rather constant and greater than that of the cluster. This dynamics, typical in this range of energy and timescale, gives rise to a variance which is not linear in time. In the inset (c) we plot the time evolution of the mean square displacement (averaged over all the particles). We have checked, by fitting the numerical data in different time intervals, that the slope is $\alpha = 1.45 \pm 0.1$ and we report in the figure a straight dotted line with this slope for comparison. Superdiffusion becomes normal only after a cross-over time and one recovers the slope $\alpha = 1$ only at equilibrium (see ref. [4] for details).

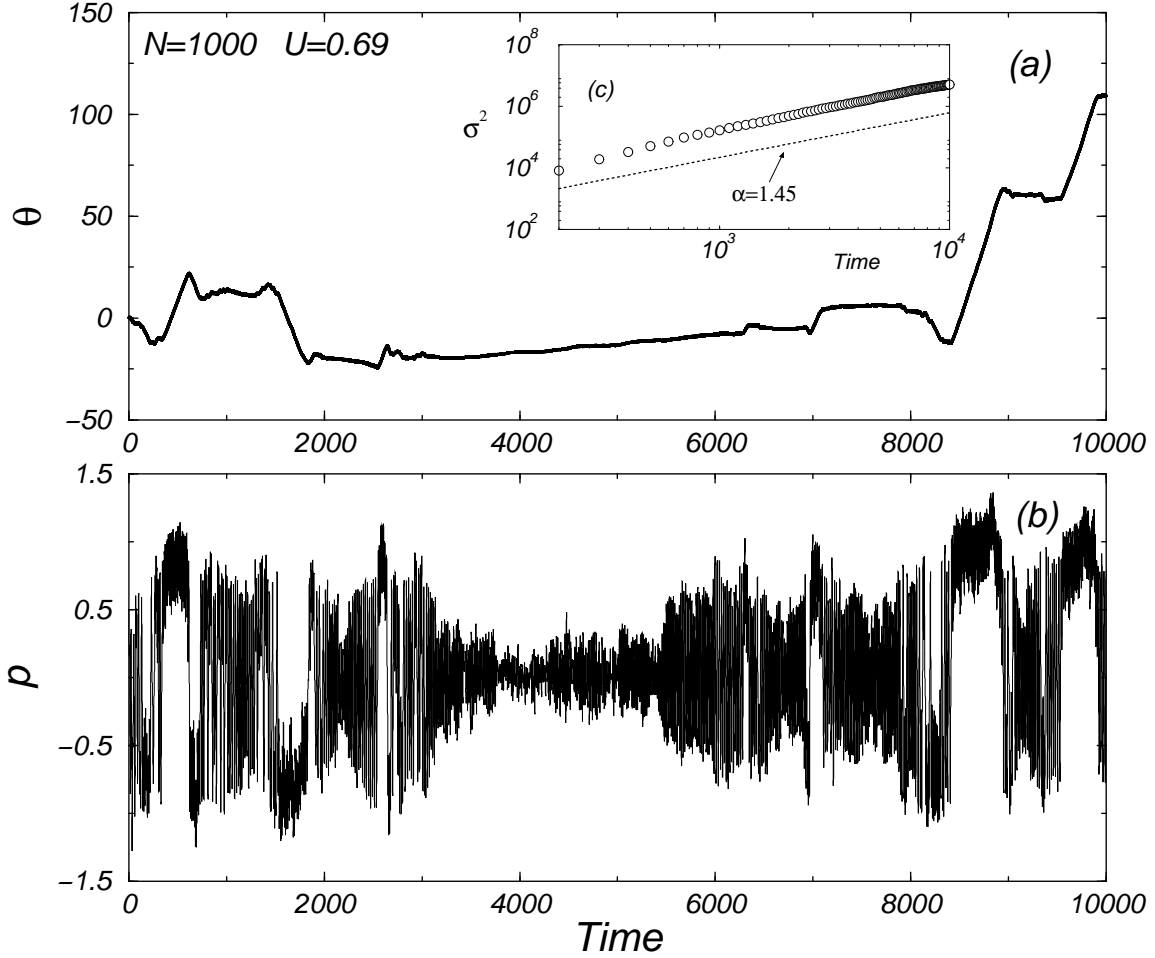


FIG. 1. Typical superdiffusion of a single particle in the transient out-of-equilibrium regime for $N=1000$ and $U=0.69$. We show the time evolution of the angle in (a) and of the corresponding momentum (b). In the inset (c) we show the behavior of the variance vs time (open symbols) and a straight dotted line with slope $\alpha = 1.45$. See text for further details.

This erratic non-brownian behavior can be better characterized by calculating the trapping times and walking times probability distributions. This study has been discussed in detail in ref. [4], where it has been shown that, using the model by Klafter and collaborators [10,13], one gets a consistent scenario of Lévy walks and superdiffusion. In fact one obtains trapping times and walking times probability distributions which are power laws, i.e.

$$P_{walk}(t) \sim t^{-\mu}, \quad P_{trap}(t) \sim t^{-\nu}, \quad (8)$$

with fitted numerical values for $U=0.69$ equal to $\mu = 2.14$, $\nu = 1.58$. These exponents, according to the Klafter and Zumofen model, obey to the formula

$$\alpha = 2 + \nu - \mu, \quad (9)$$

which gives a value $\alpha = 1.44$, consistent with the one extracted from the fit of the numerical time evolution for the mean square displacement, shown in the inset of fig.1. It has also been checked that in a region close to the critical point, from $U=0.6$ to $U=0.75$, these values do not depend in a sensitive way on the system size and only slightly on the energy density U . One has therefore Lévy walks and superdiffusive behavior, which however turns again into normal transport after a cross-over time. In Ref. [4] we have shown that this cross-over time coincides with the equilibration one.

In order to better study the non-equilibrium properties of our model, we show, in fig. 2, the time evolution of the temperature calculated through the average kinetic energy ($T = 2 \langle K \rangle / N$). We report in particular the case $U=0.69$ for different N values. The curves are the result of the averaging over ten different runs. The figure shows

that the microcanonical temperature converges to a well defined plateau, before relaxing to the canonical (greater) value, also indicated. The complete relaxation is shown only for $N=1000$, while the simulation was truncated for the other cases. This persistent and constant non-equilibrium value of the temperature, shown in the figure, indicates the presence of a dynamical Quasi-Stationary State (QSS). The simulations clearly show that the lifetime of this QSS (length of the plateaus) increases with N , and that the value of the saturation temperature converges in the continuum limit, to a particular value T_{QSS} . The latter lies on the continuation of the homogeneous canonical phase, which represents an unstable branch in the microcanonical ensemble [6]. We show in the inset of the figure the comparison between the canonical caloric curve (full curve) and the plateau temperature for $N=20000$ (open circles). In fig. 3 we compare the behavior of the QSS temperature as a function of N (open circles) with the canonical value of the temperature (dashed line). The difference between the two temperatures increases with the size of the system and reaches a saturation value around $N=20000$. The maximal size adopted in the numerical simulations was $N=25000$. The results shown in figures 2 and 3 indicate a divergence of the QSS lifetime in the limit $N \rightarrow \infty$ limit and a convergence of the microcanonical temperature to a value lower than the canonical one. In other words, in the continuum limit the system does not relax to the standard canonical equilibrium and remains forever in the QSS with a temperature T_{QSS} . The nature of these states seems to be purely dynamical and connected to a particular initialization. Further numerical investigation is in progress in this respect. From the analytical point of view, it has been shown by Ruffo at this conference, that these states correspond to a local minimum of the free energy [6].

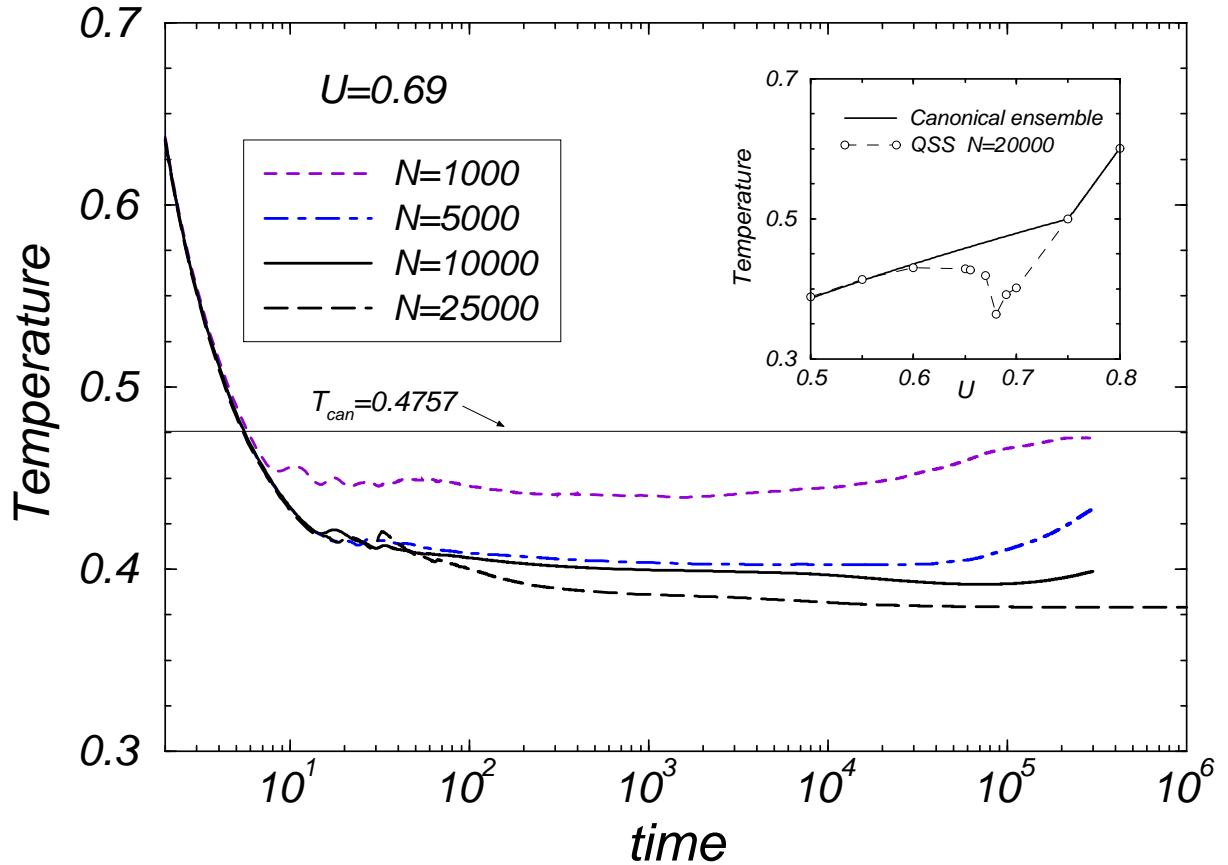


FIG. 2. Time evolution of the temperature for different systems sizes. Each curve is the result of an average over ten runs. A plateau, which increases with N exists before equilibration to the canonical ensemble. The latter is shown only for $N=1000$. We show in the inset the equilibrium caloric curve (full curve) and the out-of-equilibrium one (open symbols) calculated for $N=20000$. The latter corresponds to the value of the dynamical plateaus for different energies.

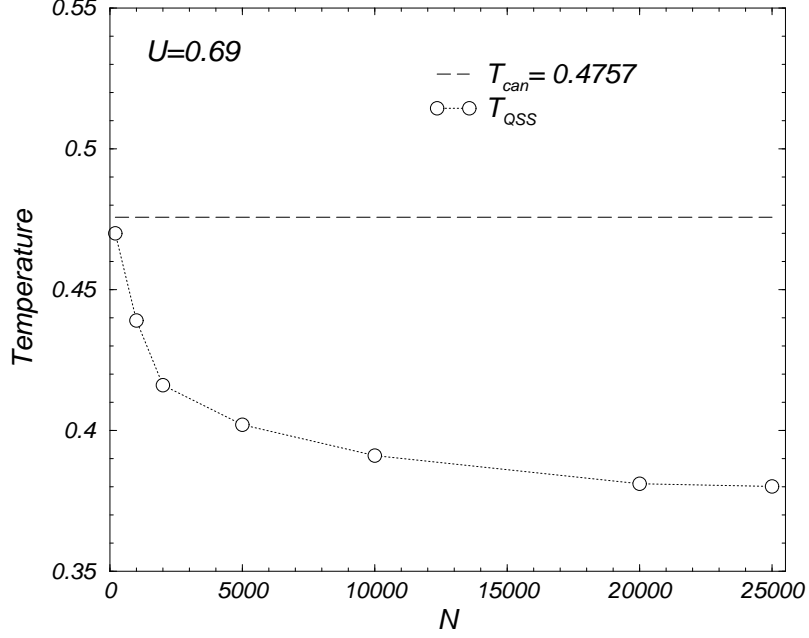


FIG. 3. Temperature of the Quasi Stationary State at $U=0.69$ vs N (open circles) in comparison with the canonical value $T_{can} = 0.4757$ (dashed line).

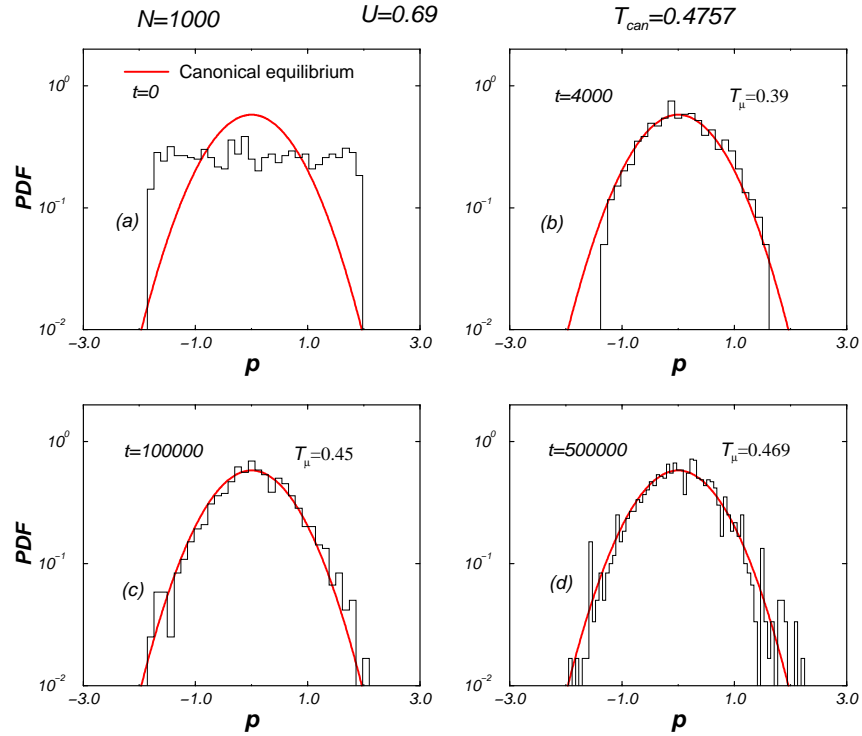


FIG. 4. The evolution of Probability Distribution Function (PDF) for the momentum at different timescales t and for $U=0.69$ (histogram) is compared with the theoretical one (full curve). Water bag initial conditions are used. The microcanonical temperatures T_μ is reported at each time for comparison. The numerical simulation shown corresponds only to one run.

Finally, we show in fig.4 the time evolution of the Probability Distribution Function (PDF) for the momentum

(histogram) at four different timescales. The case shown refers to $U = 0.69$ and $N = 1000$. Though the numerical distribution function is constructed by means of only one event and therefore is not a perfectly smooth curve, the transient regime (see in particular panel (b) at time $t = 4000$ and compare also with fig.2) shows results clearly different from the gaussian function (reported as a full curve)

$$F(p) = \frac{1}{\sqrt{2\pi T}} e^{-p^2/T} \quad (10)$$

predicted by the Vlasov solution and by the canonical ensemble [2,3]. The logarithmic scale shows that the tails of the numerical histograms are missing in the transient regime, fig.4(b), producing a microcanonical temperature T_μ (reported in the figures for each time) smaller than the canonical one $T_{can} = 0.4757$. The latter is finally reached only after a very long integration time, i.e. $t = 500000$. Preliminary and more refined results (not reported here) show a power-law decay in the tails of the QSS velocity distributions, at variance with the exponential behavior predicted by the canonical equilibrium. Summarizing, it seems that by performing the limit $N \rightarrow \infty$ before that one $t \rightarrow \infty$ the system, initialized in a water bag, will stay indefinitely out of equilibrium and the momentum distribution will never develop a Maxwellian curve. This fact seems to support the idea of C. Tsallis who suggested his generalized thermostatistics as the appropriate formalism to describe such dynamical Quasi-Stationary States [14].

IV. DISCUSSION AND CONCLUSIONS

We have presented new numerical studies on the metastable Quasi-Stationary States recently found in the dynamics of the Hamiltonian Mean Field model. HMF is an useful model to study the links between dynamics and thermodynamics in a system with long-range forces. In fact the model can be solved exactly in the canonical ensemble and this solution can be compared with microcanonical dynamical simulations for different sizes of the system.

When the microcanonical simulations are started in a out-of-equilibrium initial state, for example the so-called “water bag”, the results show a clear indication of the presence of QSS, in a transient temporal regime before relaxation. We have shown that the temperature of QSS reaches a well defined value in the continuum limit and that the lifetime of these states increases with N . Moreover the velocity distributions of QSS do not show Maxwellian tails. The corresponding caloric curve lies below the canonical one, showing a well defined backbending. The latter simulates a first order phase transition, at variance with the second order one obtained at equilibrium. Superdiffusion and Lévy walks are present in this transient out-of-equilibrium regime, for energies close to the critical one, implying a coexistence of a liquid (clustered particles) and a gas (free particles) phase. It has also been found that the cross-over time from anomalous to normal diffusion coincides with the relaxation time. The fact that the relaxation time diverges with N , though the dynamics is strongly chaotic in this region, independently on the size, is rather counter-intuitive and still not fully understood. This behavior is probably due to the fact that the greater the number of particles considered in the system, the stronger are the correlations in the dynamics. Close to the critical point, when the initial big cluster (in a water bag, all the particles are on top of each other at initial time) tries to fragment into smaller clusters, relaxation is probably hindered by these smaller fragments, which try to capture the free particles and form dynamical barriers. This effect of course increases with N .

Finally we would like to stress the similarity of the scenario indicated by our simulations with the conjecture by C. Tsallis of a different equilibrium for non-extensive systems. In fact, the HMF model, due to the long-range nature of the interaction, has a non-extensive character and shows strong correlations in space and time: the phase space is probably a multifractal in the transient regime. It is a fascinating challenge left for future investigations to study in detail the eventual connection between the out-of-equilibrium dynamics in HMF (and other similar models [15,16]) and the generalized nonextensive statistics discussed at this conference. It would be also important to study the link to real experimental systems [17,18].

This paper is part of a work in progress in collaboration with S. Ruffo and C. Tsallis.

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